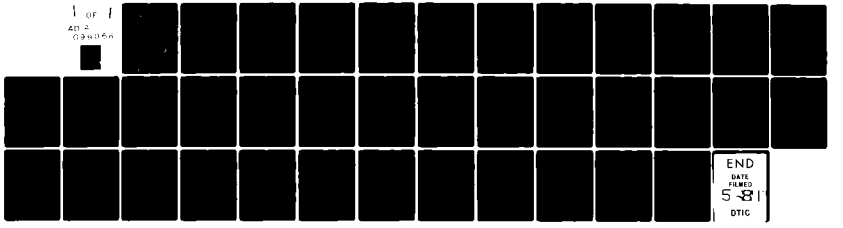
AD-A098 066 STANFORD UNIV CALIF DEPT OF CHEMISTRY F/G 7/4
THEORY AND EXPERIMENTS ON CHEMICAL INSTABILITIES.(U)
JAN 81 J ROSS AFOSR-80-0094
UNCLASSIFIED AFOSR-TR-81-0348 NL



Grant AFOSR-80-0094

Final Scientific Report

to

Air Force Office of Scientific Research

Chemistry Branch

Theory and Experiments on Chemical Instabilities

by

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11 January 1981

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFOSR-TR- 81-0348	2. GOVT ACCESSION NO. AD-A098064	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Theory and Experiments on Chemical Instabilities		5. TYPE OF REPORT & PERIOD COVERED Final 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) John Ross		8. CONTRACT OR GRANT NUMBER(s) AFOSR-80-0094
9. PERFORMING ORGANIZATION NAME AND ADDRESS Stanford University Department of Chemistry Stanford, CA 94305		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F 2303/B1
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Office of Scientific Research/NC Bldg. 410, Bolling AFB, DC 20332		12. REPORT DATE January 1981 13. NUMBER OF PAGES 35
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Franck-Condon
Adiabatic Collisions
Nonadiabatic Collisions
Stochastic Theory of Nucleation
Statistical Mechanics
Stationary States
Kinetic Instabilities

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The Franck-Condon approximation of treating an electronic transition in a molecular system at fixed nuclear coordinates is shown to provide qualitatively correct predictions. The theory was applied to both adiabatic and nonadiabatic collisions. So far only relative rates have been calculated and the challenge of predicting absolute rates remains open. A stochastic theory of nucleation in phase transitions has been developed in which the equivalence of a thermodynamic and kinetic formulation of critical cluster sizes is shown. Suitable

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use of a combination of a master equation and a form of transition probability according to Langer has been shown to lead to a most probable evolution in time which is in fact the deterministic rate equation. An extensive investigation of the formal theory of statistical mechanics of stationary states has begun. One finds that in a large system there exists subsystems which are in nonequilibrium stationary states. As a consequence, new work in the area of chemical instabilities was initiated. Topics addressed included relative stability in reactive systems far from equilibrium, chemical waves, kinetic instabilities and hydrodynamic instabilities. The interaction of chemical reactions in hydrodynamics, particular by photo-induced reactions, may be of importance in studying instabilities occurring in the atmosphere. A CARS laser apparatus has just been designed for the measurement of chemical concentrations as a function of time and spatial variables. New work on chemical instabilities using this apparatus will be funded by AFOSR.

Summary of Progress in Research

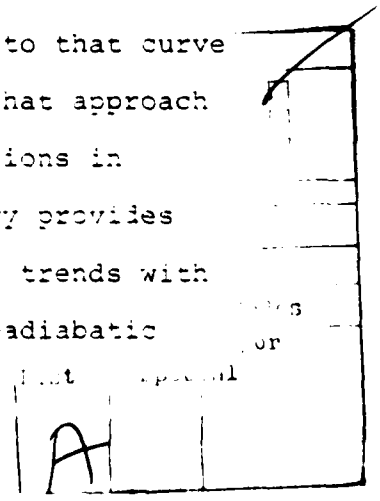
December 1976 to December 1980

Substantial progress has been made in four main areas of research sponsored by AFOSR. The numbers appearing in the text refer to the Publication List at the end on which AFOSR supported research is indicated by an asterisk.

A. Chemical Dynamics.

1. Franck-Condon approximation in chemical kinetics.

The Franck-Condon approximation of treating an electronic transition in a molecular system at essentially fixed nuclear coordinates has a basic physical similarity to the chemist's intuitive and useful notion of thinking about bond rearrangements during the chemical reaction without explicit analysis of the nuclear motion. We have studied this approach in some detail in connection with relatively simple chemical rearrangement reactions. We begin with the formal theory of scattering in which the reaction cross section is expressed as the square of a transition matrix. For reactions which occur on a single adiabatic potential surface, we recast the problem as an electronic curve crossing of two quasi-adiabatic (diabatic) surfaces and apply the Franck-Condon approximation to that curve crossing. In prior work we showed the utility of that approach by calculating rotational and vibrational distributions in the reactions $F + H_2$, D_2 and $H, D + Cl_2$. The theory provides qualitatively correct results and gives the correct trends with energy surface. We then applied the theory to non-adiabatic



collisions (133). Computationally simple, analytic formulas are developed to describe the energy dependence of quenching of electronically excited atoms by atoms and molecules. These formulas include the dependence of the Franck-Condon factors on the translational wavefunctions as well as the wavefunctions for the internal degrees of freedom. We use these formulas to evaluate the translational energy dependence of the fine structure transition cross sections for $F(^2P_{3/2}) + X \rightarrow F(^2P_{1/2}) + X$, where X = Xe, H^+, and H_2. The cross sections generally increase as the initial translational energy increases. Our results agree semiquantitatively (or better) with those obtained from other theoretical techniques. In the case of $F + H^+$ we find that the absolute cross section is sensitive to the analytic form used for the nonadiabatic coupling but our model gives the correct energy dependence. At the energies of our calculations we find only a small amount of vibrational excitation of H_2. Finally, we use our expressions to interpret some trends of available experimental results on the quenching of Hg ($^3P_2 - {}^3P_1$) by several molecules. We find that collisional excitation of the internal modes of the molecule becomes more important as the initial translational energy increases. However, these modes do not contribute to the quenching cross section in a statistical fashion.

We have used the Franck-Condon theory to calculate planar and three-dimensional angular distributions for the reaction products of atom-diatom chemical reactions (147). After applying

the Franck-Condon approximation we consider the limits of weak and strong potential coupling in the limits of weak and strong kinematic coupling. For assumed LEPS surfaces of the systems $H + H_2$, $H_2 + F$, and $H + Cl_2$, we calculate angular distributions of reaction products in the various coupling limits for ranges of final product states. Angular distribution in the strong potential coupling limit have a Gaussian shape peaked about the backscattering angle. For $H + H_2$ we find our results in the strong potential limit to be in qualitative agreement with exact quantum mechanical calculations. Angular distributions for a given product state broaden as the initial relative kinetic energy is increased in agreement with classical trajectory calculations ($F + H_2$). The angular distribution is also predicted to broaden as the final relative velocity increases, in agreement with experiment ($H + Cl_2$, $F + H_2$). We next introduce several further simplifying approximations and find that for exothermic reactions like $F + H_2$ the radial contribution to the T matrix is dominated by certain features of the potential: the barrier height, the slope of the potential on the reactant side and force constants in the region of maximum overlap. Our analysis provides a basis for the formulation of reduced variables which may be of use in comparing different reactions. Finally we discuss some sufficient conditions for the separability of product velocity and angular distributions (147).

We have thus shown that the Franck-Condon approach, based on simple, intuitive approximations, provides qualitatively

correct predictions, simply. So far only relative rates have been calculated and the challenge of predicting absolute rates remains open.

2. Molecular Beam Research

Angular and translational energy distributions have been measured for the $BaCl^+$ and Cl^- products of the reaction Ba + Cl_2 in crossed molecular beams. A center of mass (cm) cross section was derived by fitting an assumed functional form of cm to the observed laboratory (lab) scattering data. The cm behavior suggests a strongly coupled collision which contrasts with the dynamics of the neutral product channel BaCl + Cl. The threshold energy for reaction is (0.15 ± 0.05) eV. A reaction mechanism is proposed involving small impact parameter collisions with a crossing from the reactant to product surfaces occurring at the inner repulsive part of the potential. This work terminates 24 years of molecular beam research in our laboratory (156).

B. Statistical Mechanics

1. Stochastic Theory of Nucleation.

We have developed a stochastic theory of nucleation in phase transitions in which we first show the equivalence of a thermodynamic and kinetic formulation of critical cluster sizes. We use a master equation and a form of transition probability proposed by Langer to show that that combination leads to a most probable evolution in time which is in fact the deterministic rate equation. This is done by use of Feynman path integral techniques. The Langer postulate for the transition probability in the master equation is justified with reasonable approximations by means of

a derivation for the model of an Ising lattice. The stochastic formulation with path integral methods is then used to show the common origin of two different transport equations; one the Landau-Ginsburg equation, the other the Cahn-Hilliard equation. The latter is obtained when a condition of conservation of particles is proposed and the former results on relaxation of that constraint. This work, and other related research (136), has been reviewed in an invited paper (151).

2. Dynamics of Domain Walls in Ferrodistortive Materials.

We have used some results from the theory of propagation of discontinuities in systems with chemical instabilities for the purpose of an analysis of the motion of domain walls in ferrodistortive materials. Below a critical temperature ordering occurs in such systems and within a given material domains of ordered and disordered material can coexist. On application of external fields the boundaries separating the ordered and disordered domains move. We have constructed a stochastic theory for such systems which improves upon previous work by inclusion of an appropriate dissipative mechanism which assures the asymptotic attainment of a finite velocity of domain wall propagation. We start from a generalized Langevin equation of motion for the movements of the ions, which includes dissipative terms and external fields, in addition to anharmonic and strain force terms. We obtain large and small amplitude solutions corresponding to domain walls and the usual soft mode phonons, respectively. We show that apart from translation the domain walls are absolutely stable solutions

of our equation and that in external fields they reach a unique terminal velocity. The linear dependence of the velocity on the field allows us to define a temperature dependent mobility which is related to the diffusion coefficient for the wall. Furthermore, we calculate analytically the dynamic structure factor, necessary for light scattering, due to domain walls and soft-mode phonons. We find that the Brownian motion of the domain walls leads to a very narrow Rayleigh peak.

We have applied the theory just outlined to the uniaxial displacive ferroelectrics $Pb_5Ge_3O_{11}$ and SbSI. We show that the parameters necessary for our theory can be determined from available experimental data for these substances. The values so obtained are physically reasonable. With no adjustable parameters we calculate the wave number, temperature and pressure dependence of the low temperature central light scattering peak for these materials, the density of domain walls and the polarization switching time. The theoretical results agree quantitavely with the experimental data. We predict the as yet unmeasured temperature-dependent wall diffusion coefficient and the mobility of domain walls in a field.

Ferroelectric materials are important components of many electronic and computer systems.

This work has been written up in two articles and has been published in Physical Review B (144, 145).

3. Statistical Mechanics of Stationary States

We have begun an extensive investigation of the formal theory of statistical mechanics of stationary states. We begin

with the equation for a large system and show how a part of that large system, called sub-system, may exist in a quasi, nonequilibrium stationary state. We find that the fluctuations around this nonequilibrium stationary state are qualitatively different from equilibrium fluctuations and from fluctuations calculated with a local equilibrium assumption. There appears coupling between the fluctuations and the macroscopic dissipative fluxes; the coupling is due to breaking of time reversal symmetry. We derive the dynamic structure factor of importance in light scattering for a simple fluid under a temperature gradient and find this factor to consist of three terms: the first is the one predicted by local equilibrium theory and is even in wave vector and frequency; the second term is even in frequency and odd in the wave vector; and the third term is odd both in the wave vector and the frequency. We discuss possible light scattering experiments to measure the newly predicted effects (143).

C. Chemical Kinetics

We have studied the kinetics of aerosol formation in mixtures of NO_2 and SO_2 irradiated with 488 nm light which excites NO_2. The photoinduced rate measurement exceeds the thermal rate of aerosol formation. The observations are consistent with a postulated mechanism in which excited NO_2 reacts with itself and with SO_2 in the initial steps in the formation of large particles (128).

D. Chemical Instabilities

1. Stability and Relative Stability in Reactive Systems Far-from-Equilibrium

We have proposed a thermodynamic and kinetic analysis of stability and relative stability of chemical systems, far from equilibrium, which have multiple stationary states (126, 127). For given macroscopic kinetic equations we postulate that there exists an entropy state function which is maximum for the time-dependent solutions, that is concentrations of chemical species as a function of time of the kinetic equations. From that postulate we derive thermodynamic equations of motion which follow from a thermodynamic variational principle for the power dissipation and are consistent with the given kinetic equations. From the thermodynamic equations of motion we obtain necessary and sufficient conditions for stability, marginal stability, and relative stability of stationary states. The kinetic analysis is based on a stochastic approach in which we take fluctations into account. We use the theory of mean first passage time which gives a measure for the tendency of transition from one stationary state to another. For one variable and effectively one-variable systems we can find analytic results which are in qualitative agreement with those of the thermodynamic analysis. We show that in the thermodynamic limit relative stability is determined only by the properties of the stationary states. For systems with large fluctuations the assumption of an entropy state function which is maximum appears to be too restrictive and not generally applicable. The presence

of fluctuations affects measurements of relative stability, and the statistical approach appears necessary. Much future work is necessary in this area in order to arrive at a thermodynamic and statistical formulations for systems far from equilibrium.

2. Chemical Waves

The combination of nonlinear chemical reaction mechanisms and transport processes may bring about the occurrence of a variety of chemical waves. In Ref. 132 we presented a theoretical analysis of relaxation oscillation waves in which both kinetics and transport processes take place on slow and fast time scales. Such waves are known to occur not only in chemical systems but also in biological systems and certain solid state devices. We have presented a theoretical analysis based on multiple time scale procedures and the lowest order approximation provides a useful picture for such waves.

3. Kinetic Instabilities and First-order Phase Transitions

We have investigated (135) the kinetics of first-order phase transitions and find that after initial nucleation instabilities may appear in the aging stage of the phase transition, such that macroscopic structures may be formed. In prior work we have shown that such structures do in fact arise in experiments in which no gradients are present (no gradients of concentration or temperature or external forces such as the gravitational field). We present both a deterministic and statistical analysis of the problem. The essential autocatalysis necessary for the instability to occur is simply related to the fact that a large particle (as in the

phase transition leading to crystallization) is more stable than a small particle due to surface free energy terms. We perform a linear stability analysis of the kinetic equations and diffusion terms and show that the expected wave length of the pattern to be formed is in reasonable agreement with experiment. We believe that the analysis presented here is applicable to first-order phase transitions in general, provided that the time is made available necessary for the formation of spatial structures.

We have continued measurements on the formation of spatial structures in colloidal growth both in the absence and the presence of concentration gradients. The latter case is the classical Liesegang experiment. By accident we found the occurrence of spiral precipitation structures which has not been reported previously. Other experiments on such systems are reported below.

4. Hydrodynamic Instabilities.

When a fluid, gas or liquid, is subjected to a temperature gradient in the gravitational field, then convective instabilities, called Rayleigh-Bénard instabilities, may occur. We have re-investigated this much-studied problem since previous work did not consider the inclusion of cross transport coefficients such as thermal diffusion (Soret effect) and the reciprocal phenomena known as the Dufour effect. Furthermore, in much of the previous work boundary conditions applied were frequently not physically realistic. We used the hydrodynamic equations in the Boussinesq approximation and studied their stability to the onset of both

stationary and oscillatory convection. We find a variation principle for the critical Rayleigh number at the onset of stationary convection which depends on a single dimensionless parameter, a function of the thermodynamic coefficients. For certain ranges of that parameter the system becomes unstable only if heated from below. For a second range, the instability may occur only if the fluid is heated from above. For yet a third range there exists the interesting possibility of the onset of instability if the heating occurs from above or below. We also derive expressions for the amplitude of convective motion and the Nusselt number for both stationary and oscillatory convections. These expressions are then used to show that heat flux measurements may be a useful tool for the study of the onset of instability in binary fluids (148, 149).

Next we turned to the problem of the onset of convection in binary and n-component reactive mixtures in a single fluid phase (152, 153). This problem is of importance in a variety of applications. Consider, for instance, a reaction mechanism in a single phase which can become unstable and, in combination with a transport process such as diffusion or thermal conduction, can lead to the formation of spatial structures. This system can therefore also become unstable in the gravitational field and it becomes necessary to know the influence of the gravitational instability on the chemical instability. We begin our work with the study of the hydrodynamic stability of reactive, binary fluids in the Bénard geometry, and the Boussinesq approximation, with

both the Soret and Dufour effects included. The boundary conditions are rigid, perfectly conducting walls impermeable to mass flow, conditions which are experimentally approachable. For fast reactions, the reactive fluid is less stable against convection than the one-component fluid with the same values of transport and thermodynamic coefficients, due in part to the presence of a "chemical boundary layer". A slow reaction stabilizes the fluid if the heat of reaction is large and the fluctuations in temperature and concentration relax on the same time scale (gases). When the separation of these two time scales is large (liquids), reaction is always destabilizing. The influence of the Soret and Dufour effects on stability is most pronounced for slow reactions. We provide some interpretations of the role of chemical reactions on hydrodynamic stability.

Next we study the hydrodynamic stability of n-component reactive fluids undergoing a single reversible reaction in the Bénard geometry and the Boussinesq approximation, and take the Soret, Dufour and cross-diffusion effects to be negligible. The boundaries are assumed to be rigid and perfectly conducting; the dependence of the critical Rayleigh number on the assumed boundary conditions for concentrations is discussed in the limit of fast reactions. In this limit we show that, if the boundaries are impermeable to mass flow (the easiest to achieve experimentally), the critical Rayleigh number, R_∞^{cr}, is proportional to the one for nonreactive binary fluids. Apart from multiplicative factors, R_∞^{cr} depends only on a single dimensionless parameter ξ which

vanishes when all the diffusion coefficients are equal. For $\delta > 0$ (< -1) stationary convection may set in only if $R_\infty^{cr} > 0$ (< 0); for intermediate values of δ there exist both positive and negative solutions of R_∞^{cr}. This work has been published (153, 154).

The interaction of chemical reactions in hydrodynamics, particularly photo-induced reactions, may be of importance in studying instabilities occurring in the atmosphere. (For a report on the existence of multiple stationary states in a chemical reaction system in the stratosphere see M. J. Prather, M. B. McElroy, S. C. Wofsy, J. A. Logan, Geophys. Res. Lett. 6, 163 (1979).

5. Reviews of Chemical Instabilities

We have written two review articles on chemical instabilities (139, 152). In the first article we concentrate on the variety of phenomena which may occur in chemical reaction systems sufficiently far from equilibrium both in homogeneous and inhomogeneous systems. We review stability of stationary states, multiple stationary states, periodic stable oscillations, transitions between stationary and oscillatory states, chemical hysteresis, composed oscillations, the extensive variety of chemical waves, chemi-acoustic instabilities, time-independent spatial structures, and localized chemical instabilities. All of the discussion is restricted to a macroscopic treatment.

In the second review article there is some discussion of macroscopic behavior primarily for the purpose of introducing notation. The primary emphasis is on a stochastic analysis

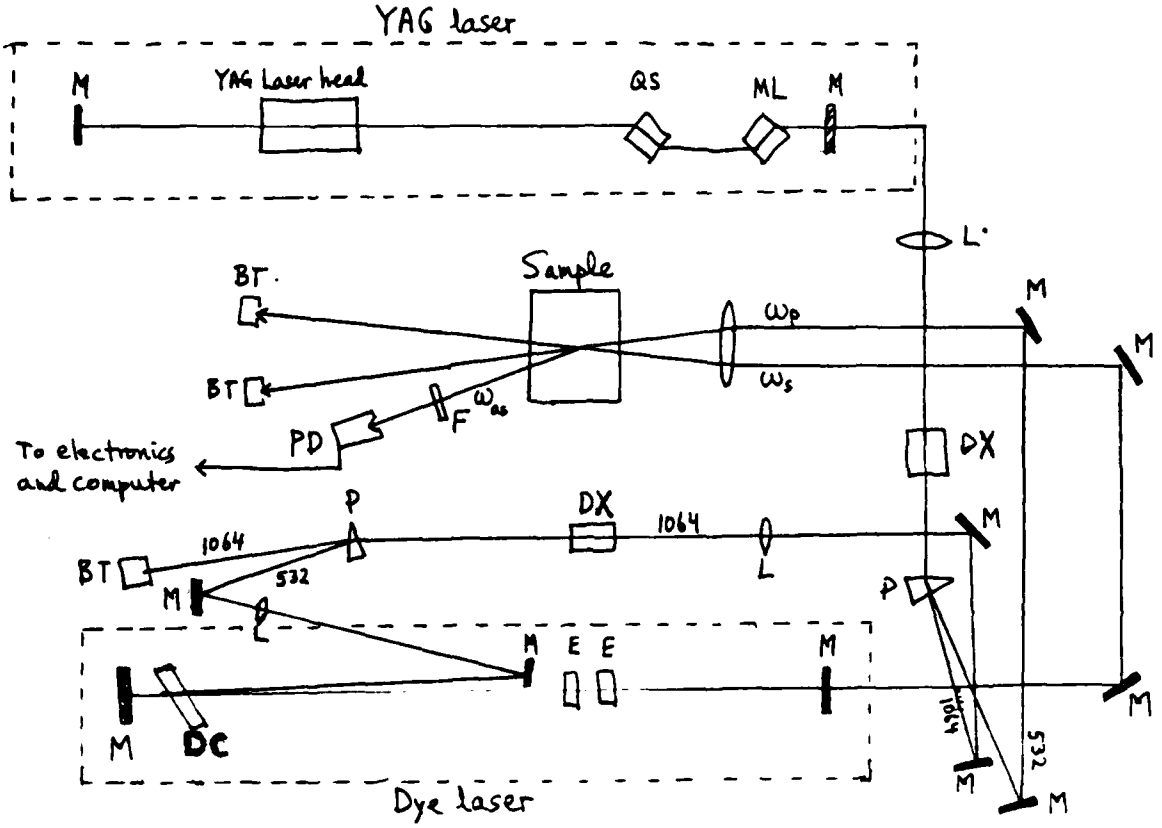
including a treatment of fluctuations in systems both near and far from equilibrium.

6. Experiments

After the relocation to Stanford we are in the process of setting up three experimental techniques for measuring various aspects of reactive systems far from equilibrium which show chemical instability behavior.

a. The first is a Vidicon photo tube for the measurement of two-dimensional profiles of chemical concentrations as a function of time. With this system we have studied the reaction $2NO_2 = N_2O_4$ driven far from equilibrium by laser irradiation. Green laser light excites NO_2 and we have predicted and observed previously the existence of multiple stationary states and hysteresis. A dilute solution of dimethyl anthracene in chloroform upon irradiation with weak light (260 nm) shows oscillatory fluorescence (in the range of 460 nm). In addition, in this system we have observed peculiar types of waves which eminate from the irradiated region. The Vidicon system is now being reassembled and is being used for the study of chemical waves and the presence of inhomogeneities in transition from one stationary state to another.

b. During the present AFOSR grant year we received funds for the construction of a CARS laser system designed for the measurement of chemical concentrations as a function of time and spatial variables. After a thorough preliminary study, we decided to assemble a system with a variety of measurement capabilities (Fig. 1).



CARS Spectrometer

M = mirror; QS = Q-switch; ML = mode locker; L = lens; DX = doubler crystal; P = prism; BT = beam terminator; DC = dye cell; E = etalon; F = filter; PD = photodiode. ω_p = pump frequency (532 nm); ω_s = Stokes-shifted frequency; ω_{as} = anti-Stokes shifted frequency.

Fig. 1

The lasers for the CARS spectrometer system are a cw-pumped acousto-optically Q-switched and mode-locked Nd-YAG laser (based on a Holobeam 258 T head and power supply) and synchronously-pumped dye laser. The YAG output at 1064 nm is typically 0.05 - 0.10 mJ in 100 psec pulses (0.5 - 1 MW) with about 20 pulses in a train each separated by 5.7 nsec; the maximum repetition rate of the pulse trains is about 1 kHz. The dye laser pulses are about 70 psec, and conversion efficiency from 532 nm is about 25%. The shot-to-shot fluctuations in power are less than 1% in the YAG, and 1-2% in the dye. The CARS signal is detected with a fast photodiode, read by a sample-and-hold circuit, and stored in a MINC-II computer. The MINC computer was purchased with funds provided by Stanford. Beam splitters and photodiodes (not shown) also detect a small portion of the input beams to provide a reference signal for greater precision. For measurements at different spatial points simultaneously, Pockel cell modulators in the input beams may be used to direct the light into one of two focussing lenses, with a modulation period short compared to relaxation times in the sample. In addition, the input beams are essentially undepleted and may be focussed back into the sample at a different point. The parts for the laser system have been ordered, have arrived, and have been assembled. The YAG laser has been tested and operates satisfactorily. We are in the process of our first measurements on the NO_2-N_2O_4 system.

The system is designed to provide the possibility of CARS measurements; stimulated Raman-gain measurements and other

region of multiple stationary states. Thus there is an analogy with phase transitions in which, during the transition, liquid droplets are immersed in the gas phase in a gas-to-liquid transition.

d. We have made a large number of measurements on the formation of spatial structures both in the presence and absence of external radiance. Two interesting new effects have been observed: (1) the formation of spiral structures in a standard Liesegang ring experiment; (2) the formation of structure in a Liesegang ring experiment in which there exist radial gradients where structures both in the radial and angular coordinate are found. Furthermore we have investigated the influence of gravity on the formation of spatial structures and from these measurements obtained information on the extent to which the periodic precipitation processes are determined by post nucleation phenomena.

7. Personnel

The following personnel have contributed to research discussed in this final technical report. Following the name of each person there appears in parentheses the association with the program described here and then the current affiliation.

H. Metiu (Postdoctoral Research Associate), Professor of Chemistry, University of California, Santa Barbara.

T. George (Postdoctoral Research Associate), Professor of Chemistry, Rochester University.

Itamar Procaccia (Postdoctoral Research Associate),Associate Professor of Chemistry, Weizmann Institute of Science, Israel.

David J. Zvijac (Postdoctoral Research Associate), Scientist, Center for Naval Analysis.

Shaul Mukamel (Postdoctoral Research Associate), Associate Professor of Chemistry, Rice University.

K. Iwamoto, (Postdoctoral Research Associate), Research Scientist, Kyoto University, Japan

Nathan Presser (Postdoctoral Research Associate), Research Scientist, U.S. Industries.

M.A. Collins (Postdoctoral Research Associate), Assistant Professor, National University, Canberra, Australia.

John F. Currie (Postdoctoral Research Associate), Assistant Professor of Physics, University of Montreal, Canada.

Dina Gutkowitz-Krusin (Postdoctoral Research Associate), Research Scientist, Exxon Research Laboratories.

Carlos L. Vila (Graduate Student), Assistant Professor of Chemistry, University of Puerto Rico.

R. H. Burton (Graduate Student), Research Scientist, Bell Telephone Laboratories.

Peter Richter (Research Associate), Professor of Physics,
University of Bremen, W. Germany.

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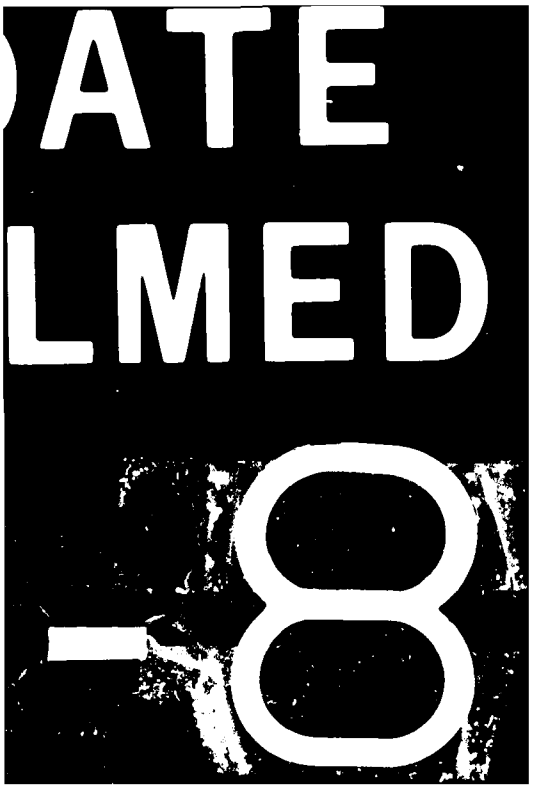
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